# APPENDIX A. SOLUTIONS FOR EXTREME VALUES

## Confidence Intervals

In this section we derive equations for extreme values of $g(\gamma\boldsymbol{\theta})$ for a linearized form of $L(\boldsymbol{\theta},\lambda)$ given by equation 8. These equations become iteration equations to solve the nonlinear problem.

First, we linearize $g(\gamma\boldsymbol{\theta})$ and $\boldsymbol{f}(\gamma\boldsymbol{\theta})$ using a truncated Taylor series around parameter set $\boldsymbol{\theta}_r$ obtained at the *r*th iteration:

$$g(\gamma\boldsymbol{\theta}) \approx g(\gamma\boldsymbol{\theta}_r) + \boldsymbol{D}g_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r), \tag{A-1}$$

$$\boldsymbol{f}(\gamma\boldsymbol{\theta}) \approx \boldsymbol{f}(\gamma\boldsymbol{\theta}_r) + \boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r), \tag{A-2}$$

where subscript *r* indicates evaluation using $\boldsymbol{\theta}_r$. Second, we take derivatives of $L(\boldsymbol{\theta},\lambda)$ written using equations A-1 and A-2 and set the results to zero to obtain

$$\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r) = \lambda\boldsymbol{D}g' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r)), \tag{A-3}$$

$$d_\alpha^2 = S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}). \tag{A-4}$$

Third, we write $S(\boldsymbol{\theta})$ using equation A-2, then substitute $\boldsymbol{\theta}-\boldsymbol{\theta}_r$ from equation A-3 into the result to get

$$\begin{aligned}
S(\boldsymbol{\theta}) &= S(\boldsymbol{\theta}_r) - 2(\boldsymbol{\theta}-\boldsymbol{\theta}_r)'\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)) + (\boldsymbol{\theta}-\boldsymbol{\theta}_r)'\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r)\\
&= S(\boldsymbol{\theta}_r) - 2(\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)))'(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))\\
&+ (\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)))'(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}(\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)))\\
&= S(\boldsymbol{\theta}_r) + \lambda^2\boldsymbol{D}g_r(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{D}g_r' - (\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))\\
&= S(\boldsymbol{\theta}_r) + \lambda^2\boldsymbol{Q}_r'\boldsymbol{Q}_r - (\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)).
\end{aligned} \tag{A-5}$$

Fourth, we put equation A-5 into equation A-4 and solve for λ to get

$$\lambda = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}\right)^{1/2}. \tag{A-6}$$

To obtain the solution for the $(r+1)$th iteration, we write equations A-6 and A-3 in the forms

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}\right)^{1/2} \tag{A-7}$$

and

$$\boldsymbol{\theta}_{r+1} = \boldsymbol{\theta}_r + \lambda_{r+1}(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Dg}_r' + (\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)). \tag{A-8}$$

## Prediction Intervals

Extreme values of $g(\gamma\boldsymbol{\theta}) + v$ are derived using the same general method as used for $g(\gamma\boldsymbol{\theta})$. First, we use equations A-1 and A-2 in equation 19 and take derivatives with respect to $\boldsymbol{\theta}, v,$ and $\lambda$. Then we set the results to zero to obtain

$$\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta} - \boldsymbol{\theta}_r) = \lambda\boldsymbol{Dg}_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)), \tag{A-9}$$

$$\omega_p v = \lambda\ , \tag{A-10}$$

$$d_\alpha^2 = S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) + \omega_p v^2. \tag{A-11}$$

Second, we use equations A-5 and A-10 in equation A-11 to get

$$d_\alpha^2 = S(\boldsymbol{\theta}_r) - S(\hat{\boldsymbol{\theta}}) + \lambda^2(\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}) - (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)),$$

from which

$$\lambda = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}}\right)^{1/2}. \tag{A-12}$$

Iteration equations are obtained directly from equations A-12, A-10, and A-9 and have the form

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}}\right)^{1/2}, \tag{A-13}$$

$$v_{r+1} = \omega_p^{-1}\lambda_{r+1}\ , \tag{A-14}$$

and equation A-8.